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Optimization and Discrete Mathematics

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Optimization and Discrete Mathematics

PM: Don Hearn

BRIEF DESCRIPTION OF PORTFOLIO:

Development of optimization and discrete mathematics for solving large, complex problems in support of future Air Force science and engineering, command and control systems, logistics, and battlefield management

LIST SUB-AREAS IN PORTFOLIO:

- Analysis based optimization
- Continuous and Discrete Search methods
- Dynamic, Stochastic and Simulation Optimization
- Combinatorial Optimization

Outline

- Portfolio Overview
- Optimization Research
- Program Goals and Strategies
- AF Future Applications Identified
- Program Trends
- Transitions
- Scientific Opportunities and Transformation Opportunities; Relation of Other Agency Funding
- Examples from the portfolio
- Summary

Optimization Research

- **Starts with an important hard problem**

- **Optimization models are proposed**

- **Theoretical properties – existence and uniqueness of solutions, computational complexity, approximations, duality, …**

- **Solution methods – convergence theory, error analysis, bounds, …**

- **If successful, generalize!**

Optimization Models

Maximize (or Minimize) f(x)

Subject to

$$g(x) \leq 0$$
$$h(x) = 0$$

where x is an n-dimensional vector and g, h are vector functions. Data can be deterministic or stochastic and time-dependent.

The simplest (in terms of functional form) is the Linear Program:

Minimize 3x + 5y + z + 6u + ……..

Subject to

$$3x + y + 2z + \ldots\ldots \quad \leq \quad 152$$
$$2x + 7y + 4z + u \ldots\ldots \quad \geq \quad 130$$
$$12x + 33y + 2u \quad \ldots\ldots = \quad 217$$

etc

Textbook Nonlinear Example

- **Local optima are a problem:**

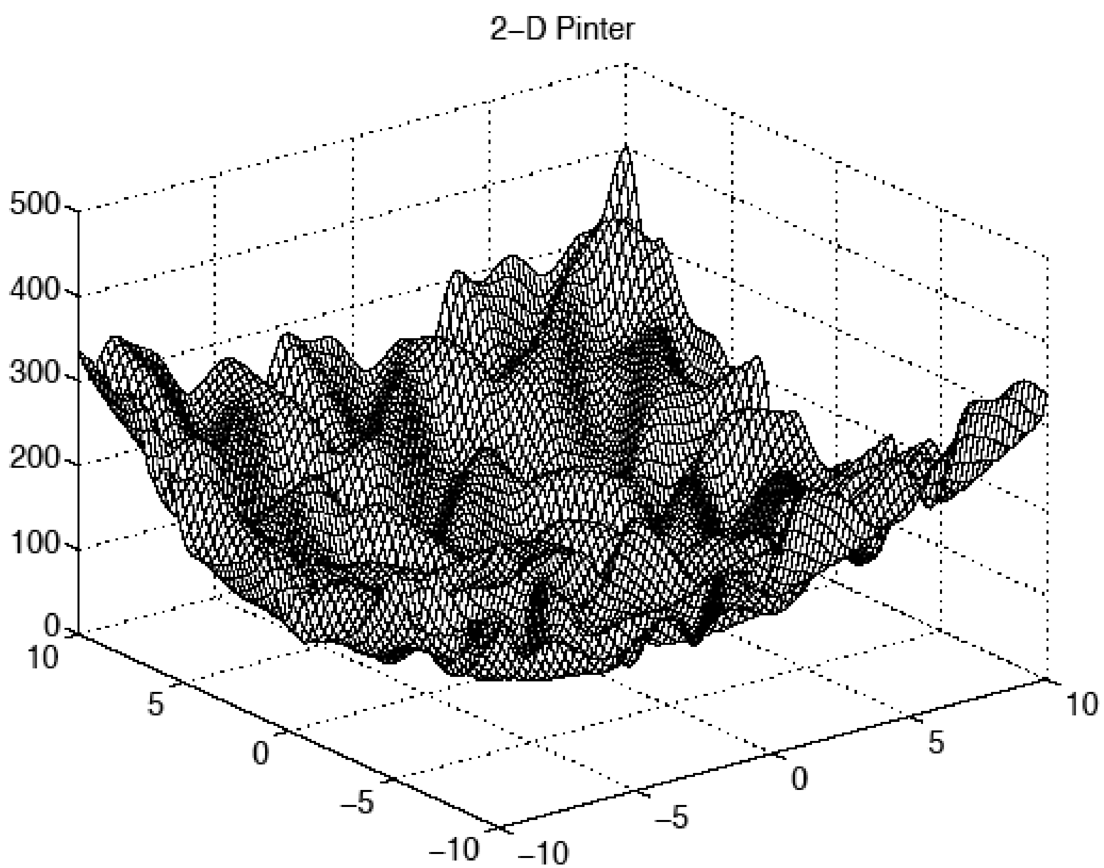


Figure 4: 2-D Pinter function, where $-10 \leq x_i \leq 10,\ i = 1, 2.$

Program Goals & Strategies

- **Goals –**
  - **Cutting edge optimization research**
  - **Of future use to the Air Force**

- **Strategies –**
  - **Stress rigorous models and algorithms , especially for environments with rapidly evolving and uncertain data**
  - **Engage more recognized optimization researchers, including more young PIs**
  - **Foster collaborations –**
    - **Optimizers, engineers and scientists**
    - **Between PIs and AF labs**
    - **With other AFOSR programs**
    - **With NSF, ONR, ARO**

Future AF Applications Identified

- **Engineering design, including peta-scale methods**
- **Risk Management and Defend-Attack-Defend models**
- **Real-time logistics**
- **Optimal learning/machine learning**
- **Optimal photonic material design (meta-materials)**
- **Satellite and target tracking**
- **Embedded optimization for control**
- **Network data mining**
- **…….. (to be continued)**

Scientific Challenges and Potential Impacts

Some Scientific Challenges

- ***Non-differentiable Optimization***
- ***Nonlinear Optimization for Integer and Combinatorial Models***
- ***Simulation Optimization***
- ***Optimization for analysis of Biological and Social Networks***
- ***Real Time Logistics***
- ***Risk and Uncertainty in Engineering Design***

Potential Transformational Impacts

- ***Meta-material design***
- ***Engineering optimization***
- ***AI, Machine Learning, Reinforcement Learning***
- ***Air Force Logistics***

Program Trends

Analysis based optimization – Emphasis on theoretical results to exploit problem structure and establish convergence properties supporting the development of algorithms

Search based optimization – New methods to address very large continuous or discrete problems, but with an emphasis on the mathematical underpinnings, provable bounds, etc

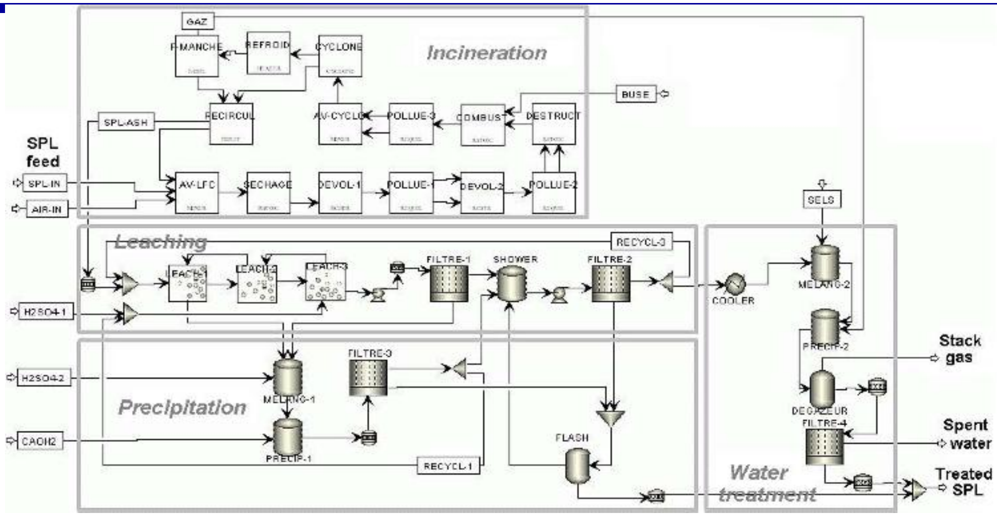
Dynamic, stochastic and simulation optimization– New algorithms that address data dynamics and uncertainty and include optimization of simulation parameters

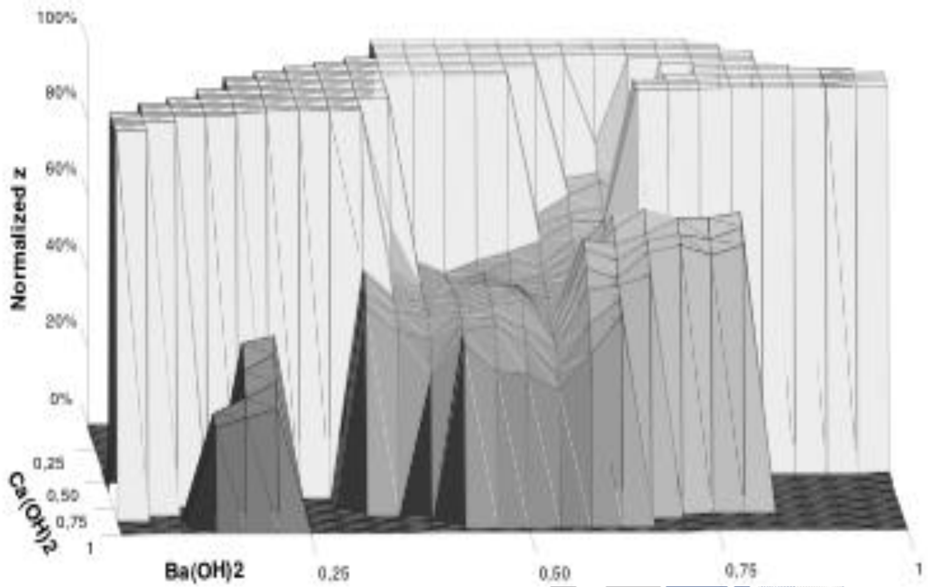
Combinatorial optimization – New algorithms that address fundamental problems in networks and graphs such as identifying substructures

Recent Transition: Model Adaptive Search for detoxification process design

Dennis (Rice), Audet (École Polytechnique de Montréal), Abramson (Boeing)

- The MADS algorithm, based on (Clarke) generalized derivatives, reduced the solution times by 37% on this problem in which expensive simulations were need to evaluate the objective function.
- Series of publications on the theory (*SIAM Optimization* + others)
- Numerous transitions

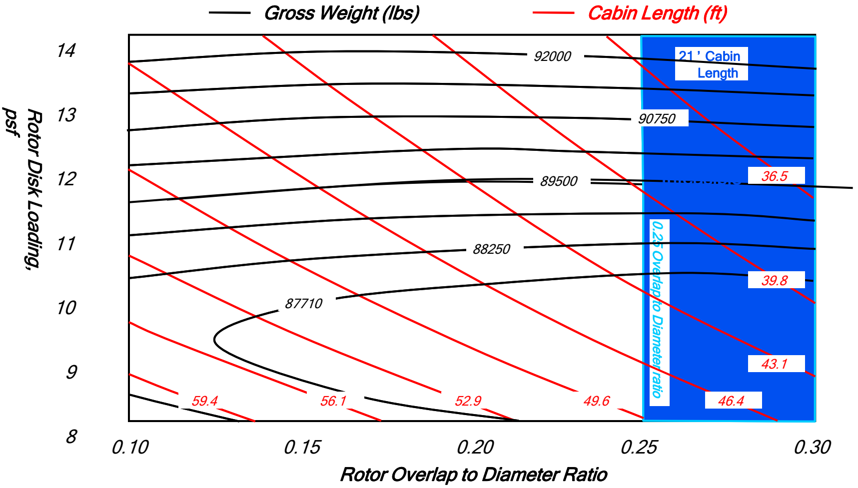


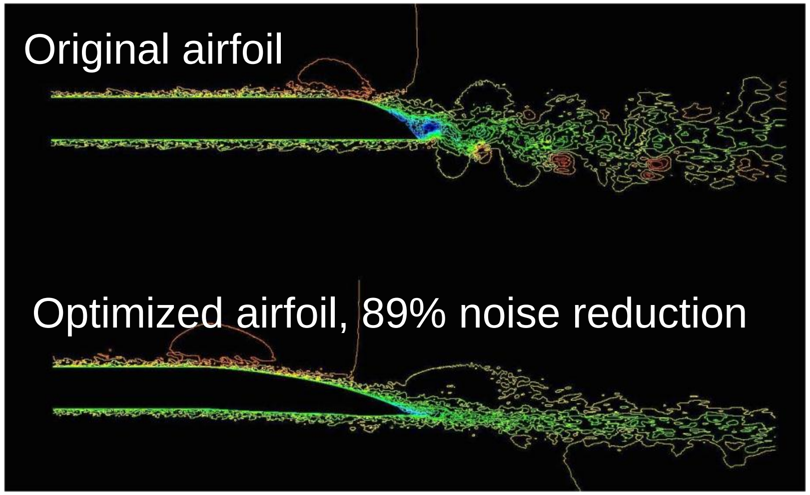


New Meta Algorithms for Engineering Design Using Surrogate Functions

Dennis (Rice), Audet (École Polytechnique de Montréal), Abramson (Boeing)

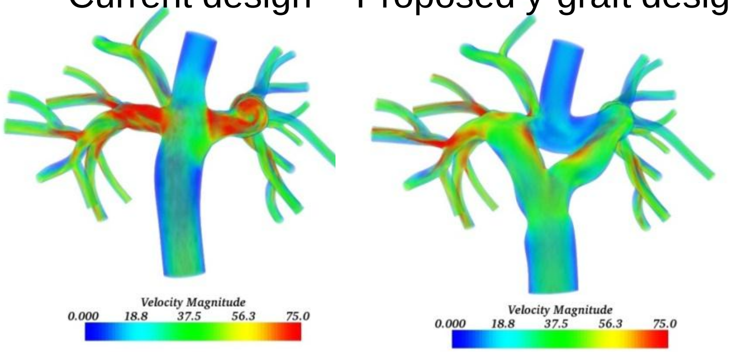
Helicopter rotor tilt design at Boeing



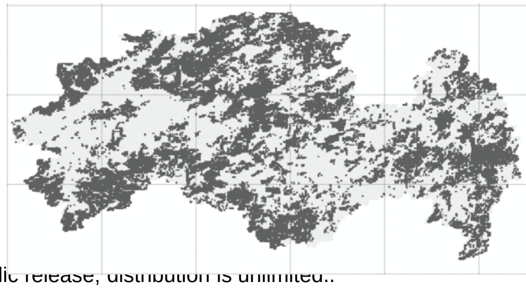


Optimization of angle and graft size for bypass surgery

Current design   Proposed y-graft design



Snow water equivalent estimation



Highly fragmented domain

Feasible domain represented by the dark pixels.

Defend-Attack-Defend Optimization Models

NPS (Joint work with ONR), Brown, Wood, et al.

"Operate-Attack-Defend" San Francisco Bridges – 3 objectives:

- **Defend: critical arcs with resources available**
- **Attack: impedes traffic flows**
- **Operate: after the attack**
- **Formulation: nonlinear D-A-D model (extended Stackelberg game)**
- **Methods: new nonlinear decomposition algorithms**
- **Model provides:**
  - **Relative importance of components**
  - **Improves on std risk analysis**
  - **Cost assessments**

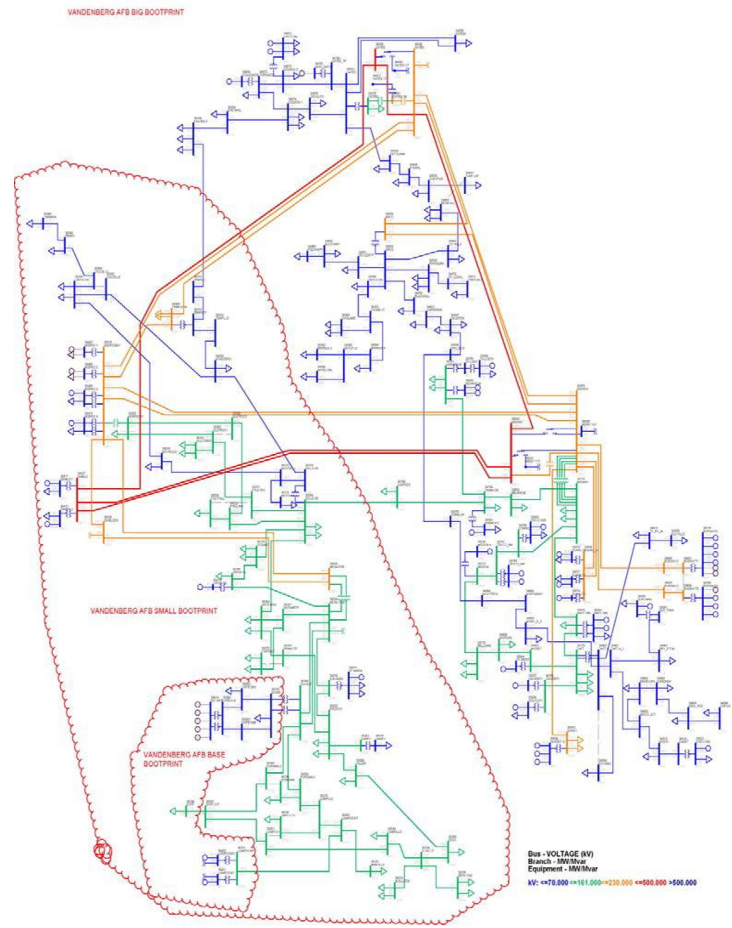
Recent Transition

RESILIENCE REPORT: ELECTRIC POWER INFRASTRUCTURE SUPPORTING MISSION ASSURANCE AT VANDENBERG AIR FORCE BASE

Javier Salmerón
David L. Alderson
Gerald G. Brown

NPS Center for Infrastructure Defense

December 2011



Other Organizations That Fund Related Work

- ***NSF***

  Several projects jointly funded in the 4 subareas
- ***ONR***
  - **3 projects (5 PIs) jointly funded – in D-A-D modeling, military logistics and stochastic optimization**
- ***DOE***
  - **No joint grants. One PI has additional funding in energy management**
- ***ARO***
  - **No joint project funding. One PI is on Army MURI**

International Collaborations

- *Ecole Polytechnique de Montreal*
  - Claude Audet (with US researchers at Rice, Boeing, AFIT)

- *University of Waterloo*
  - S. Vavasis & H. Wolkowicz

- *SOARD*
  - Claudia Sagastizabal, RJ Brazil (with R. Mifflin, Wash. St.)

(plus many unsponsored collaborations)

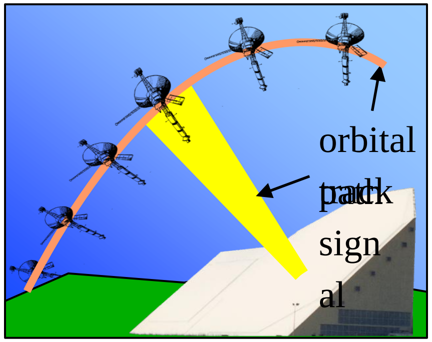
Examples from the Portfolio

Discrete Search - Theory and Methods

– **Jacobson, Howe and Whitley**

- *Study of landscapes in combinatorial problems*
- *Applications in radar scheduling, routing, general NP Hard problems such as TSP, Air Fleet assignment, homeland security, …*

Colorado State University, Howe & Whitley



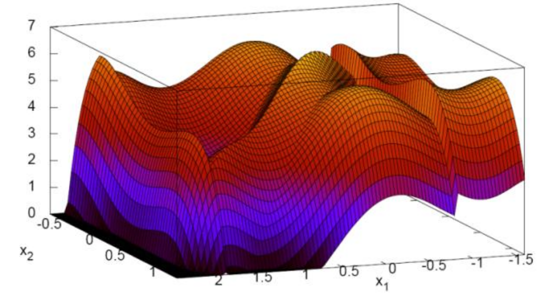
Origin - tough scheduling problems

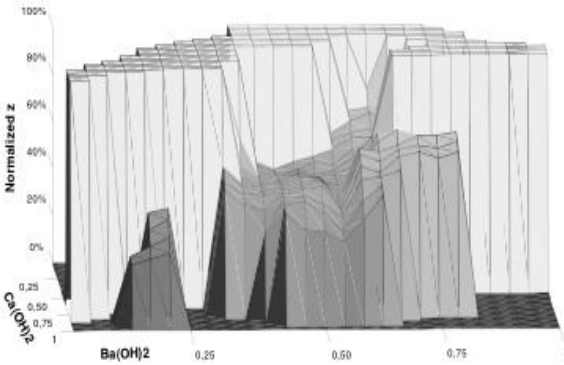
Led to new research on landscapes and TSPs

Traveling Salesman Problem (e.g., supply chain, logistics, circuit designs, vehicle routing)

- **Generalized Partition Crossover (GPX): technique for combining two locally optimal solutions to construct better locally optimal solution in *O(n)* time**
- **Results: Analytical and empirical analysis shows GPX can dominate state of the art methods**

Implications: Can dramatically change how TSP instances are solved





Optimal Dynamic Asset Allocation Problems: Addressing the Impact of Information Uncertainty & Quality

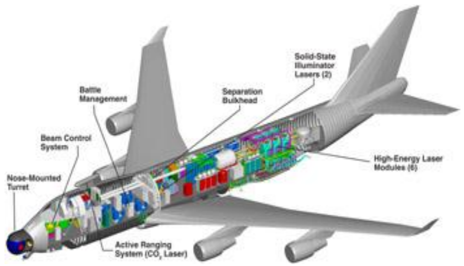
University of Illinois, Sheldon Jacobson

Goal: Create a general theoretical framework for addressing optimal dynamic asset allocation problems in the presence of information uncertainty and limited information quality.

Technical Approaches:

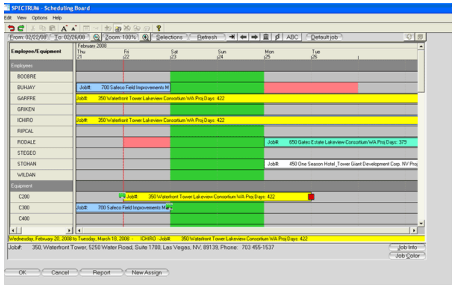
- Sequential Stochastic Assignment
- Surrogate Model Formulation and Analysis
- Dynamic Programming Algorithm Design

Applications



Assignment Problems

Screening and Protection



Scheduling Problems

Payoff to Stakeholders:

- **Theory: New fundamental understanding of how data deficiencies and uncertainties impact sequential stochastic assignment problem solutions.**
- Long-term payoff: Ability to solve problems that more closely mimic real-world systems driven by real-time data.

Analysis-Based Optimization Theory and Methods

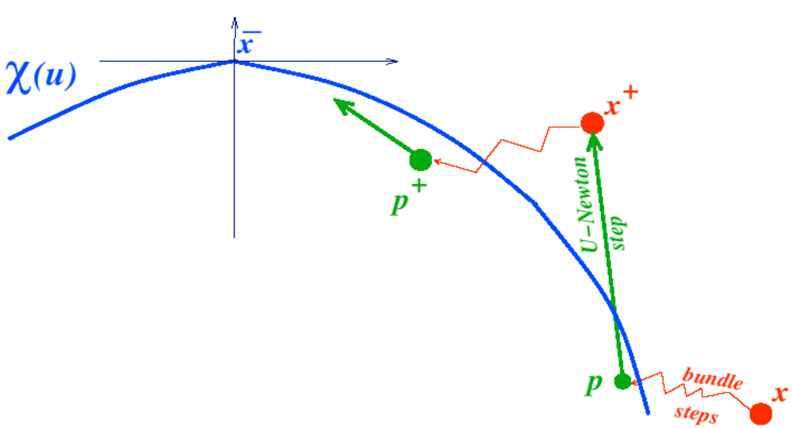
- Mifflin and Sagastizabal
  - *New theory leading to rapid convergence in non-differentiable optimization*
- Freund and Peraire
  - *SDP for meta-material design*
- Srikant
  - *Wireless Network Operation*

Breakthrough: Super-linear convergence for certain non-smooth problems

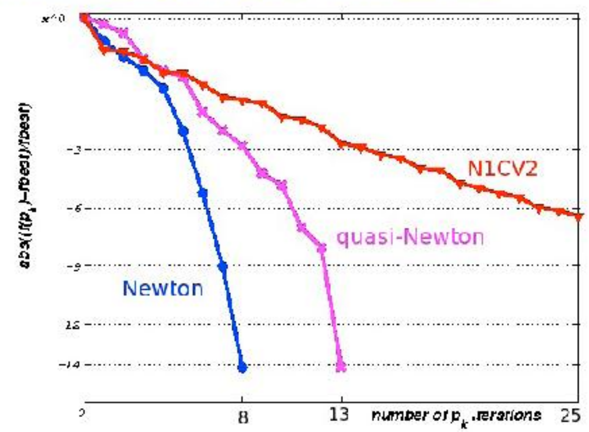
Bob Mifflin (Washington State) and Claudia Sagastizabal (CEPEL, Rio de Janeiro)

jointly supported with NSF and SOARD

0.1 Ideal iteration



Superlinear Convergence for MAXQUAD



Main ref.: A VU algorithm for convex minimization R. Mifflin and C. Sagastizábal. Math. Program. 104(2-3), pp. 583-608, 2005.

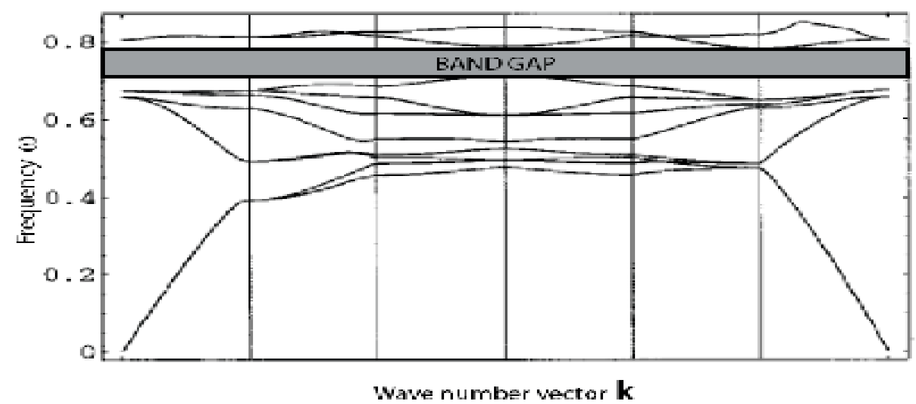
Future work: quasi-Newton, μ-adjustment, lower C^2 functions

Band-gap optimization for wave propagation in periodic media

MIT, Freund, Parrilo & Peraire

Design of materials that give very precise control of light or sound waves

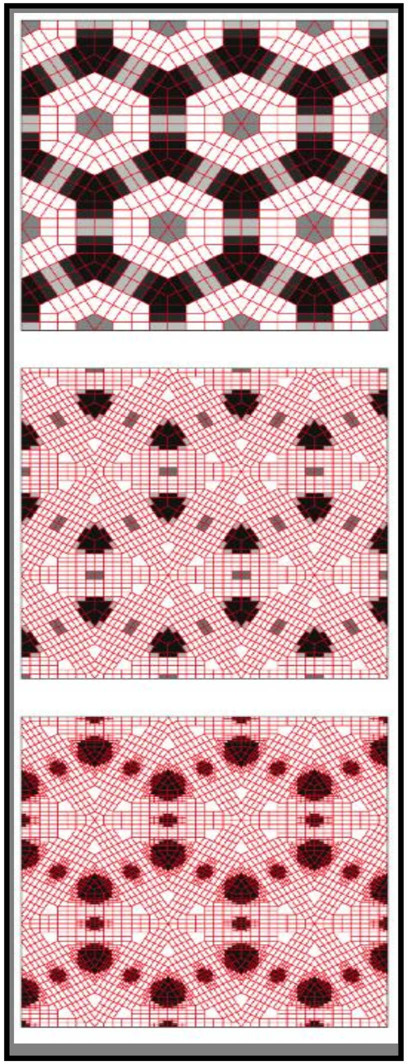
New in this work is the use of Semi-Definite Optimization for band structure calculation and optimization in phononic crystals



Applications include design of elastic waveguides, beam splitters, acoustic lasers, perfect acoustic mirrors, vibration protection devices

Optimization of photonic band gaps

MIT, Freund & Peraire



Goal: Design of photonic crystals with multiple and combined band gaps

Approach: *Solution Strategies*

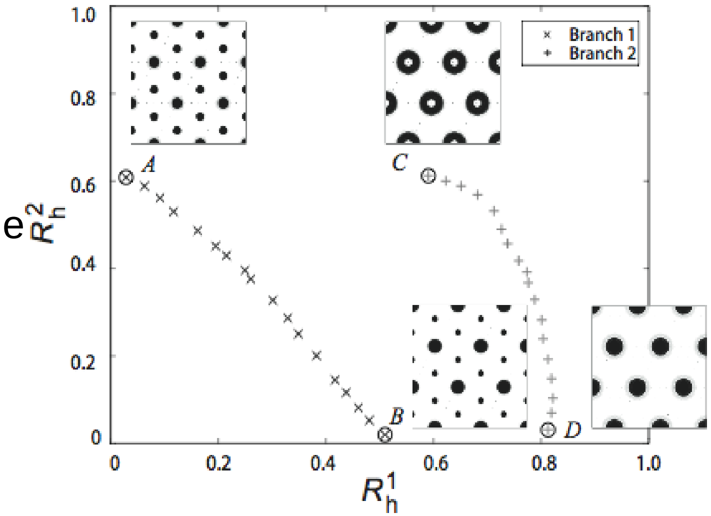
- Pixel-based topology optimization
- Large-scale non-convex eigenvalue optimization problem
- Relaxation and linearization

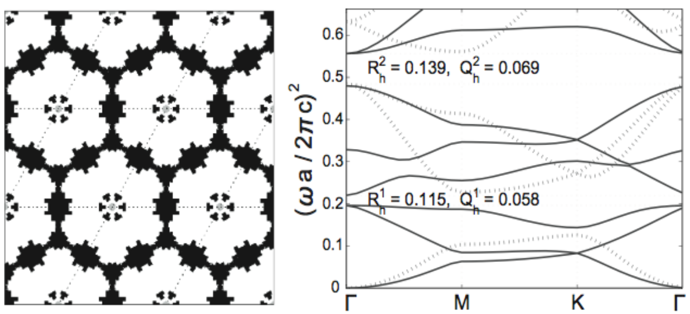
Methods: *Numerical optimization tools*

- Semi-definite programming
- Subspace approximation method
- Discrete system via Finite Element discretezation and Adaptive mesh refinement

Results: *Square and triangular lattices*

- **Very large absolute band gaps**
- **Multiple complete band gaps**
- **Much larger than existing results.**





Dynamic and Stochastic Methods

- **Stochastic Optimization –**
  - **Marcus and Fu**
    - *Simulation-based optimization*
- **Dynamic Optimization**
  - **Powell, Sen, Magnanti and Levi**
    - *Fleet scheduling, Refueling, ADP, Learning methods, Logistics*

The research challenge

- **Solve**

$$\max_\pi E^\pi \left\{ \sum_t \gamma^t C\left(S_t, X^\pi(S_t)\right) \right\}$$

given a *system model* (transition function)

$$S_{t+1} = S^M\left(S_t, x_t, W_{t+1}(\omega)\right)$$

  - **Goal: a method that reliably finds near-optimal policies for the broadest class of problems, with an absolute minimum of tunable parameters.**


Stochastic programming
Stochastic search
Model predictive control
Optimal control
Reinforcement learning
$Q-$learning
On-policy learning
Off-policy learning
Markov decision processes
Simulation optimization
Policy search

The Knowledge Gradient for Optimal Learning In Expensive Information Collection Problems

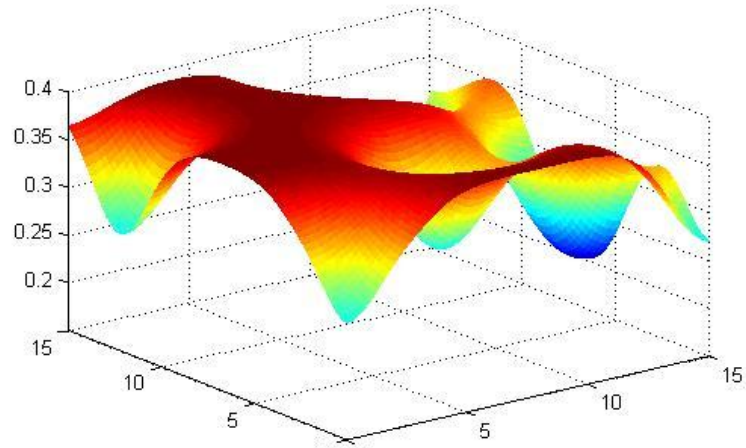
Princeton University, Warren B. Powell

Challenge

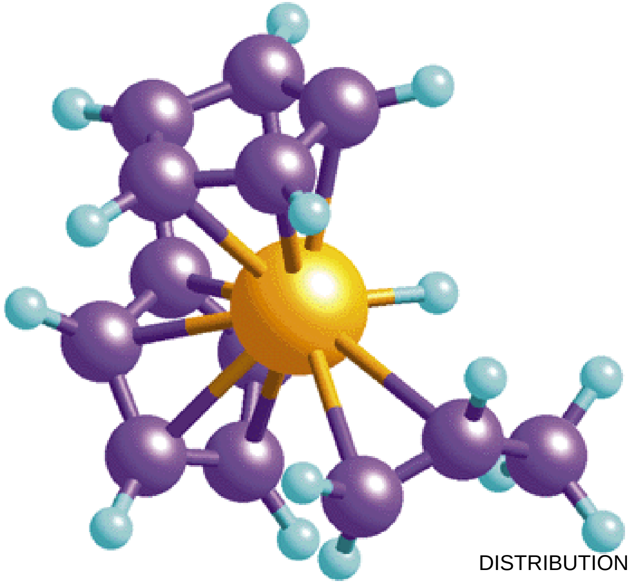
- Finding the best material, technology, operating policy or design when field or laboratory experiments are expensive.

Breakthrough

- The knowledge gradient for correlated beliefs (KGCB) is a powerful method for guiding the efficient collection of information. Proving to be robust across broad problem classes.



A knowledge gradient surface



Technical challenge

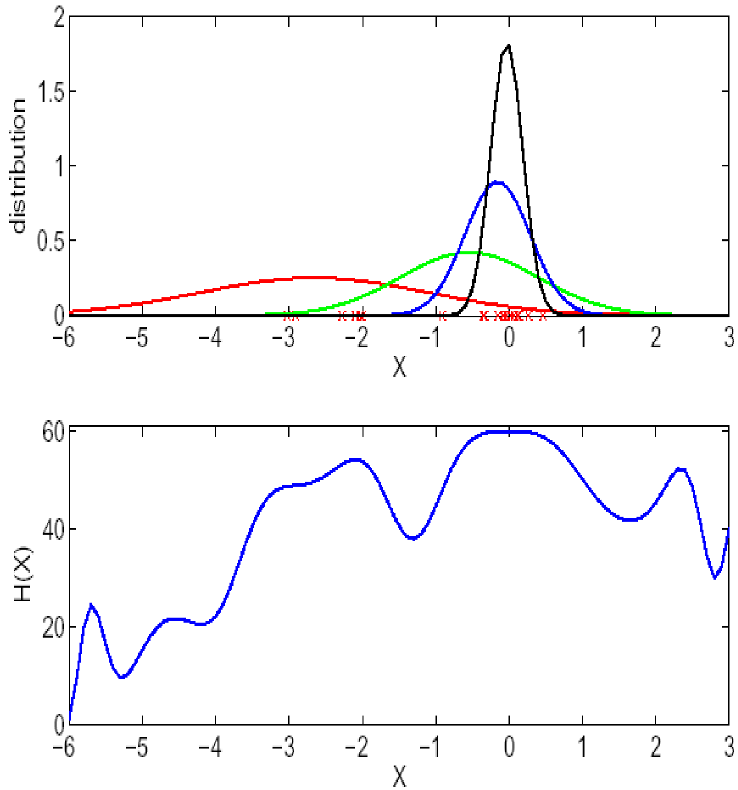
- Optimal information collection policies are computationally intractable.
- Efficient algorithm for capturing correlated beliefs, making it possible to solve problems with thousands of choices on small budgets.

Impact

- Used to find new drugs, improve manufacturing processes, and optimize policies for stochastic simulators.

UMD (with NSF), S. Marcus & M. Fu

Convergence of Distribution to Optimum in Simulation-Based Optimization



ACCOMPLISHMENTS

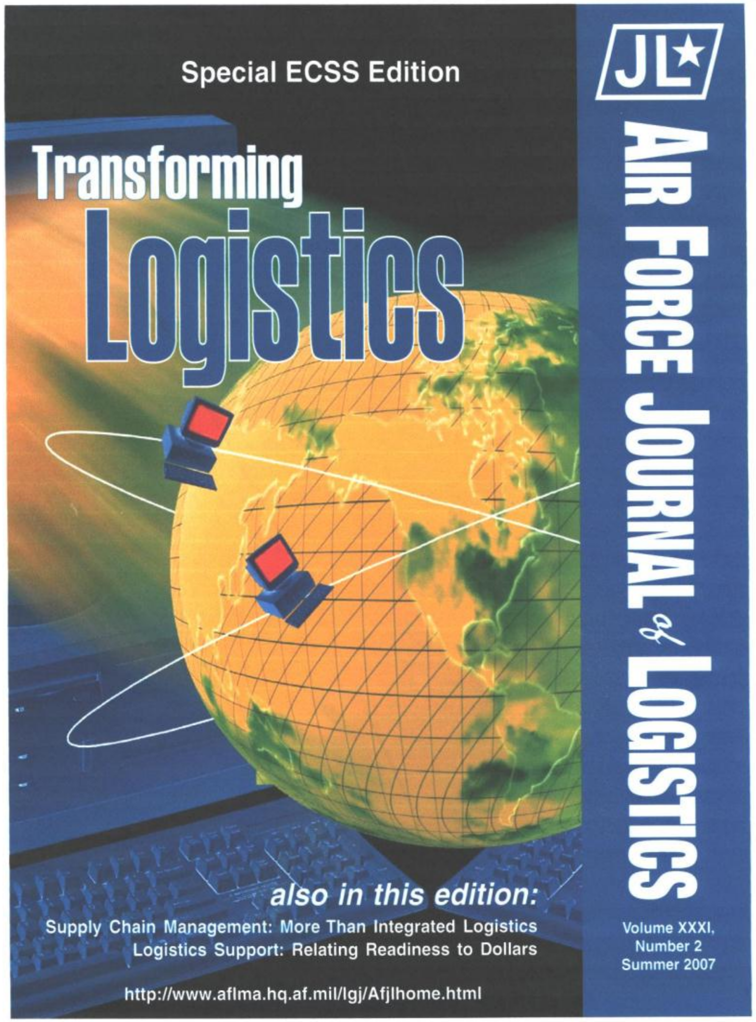
- **Simulation-based optimization algorithms with probable convergence & efficient performance**

- **Evolutionary and sampling-based methods for Markov Decision processes**

An Optimization Framework for Air Force Logistics of the Future

MIT, Magnanti & Levi

- **Air Force Logistics –**
  - **20 new initiatives to revolutionize supply chains and logistics**
- **DOD logistics + inventory costs**
  - **$130 + $80 billion**
- **Magnanti and Levi (MIT) - fast real-time algorithms for**
  - **Depot to base supply and joint replenishment**
- **Future war space example - sensor asset allocation**
- **Workshop in 2010 on identification of specific AF models for the future**



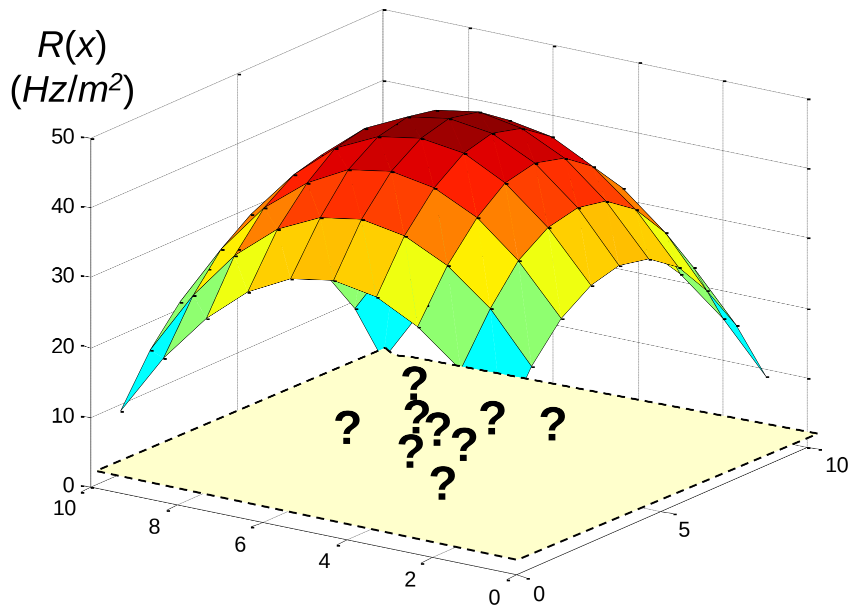
OPTIMAL COVERAGE PROBLEM:

Deploy vehicles/sensors to maximize "event" detection probability

– unknown event locations

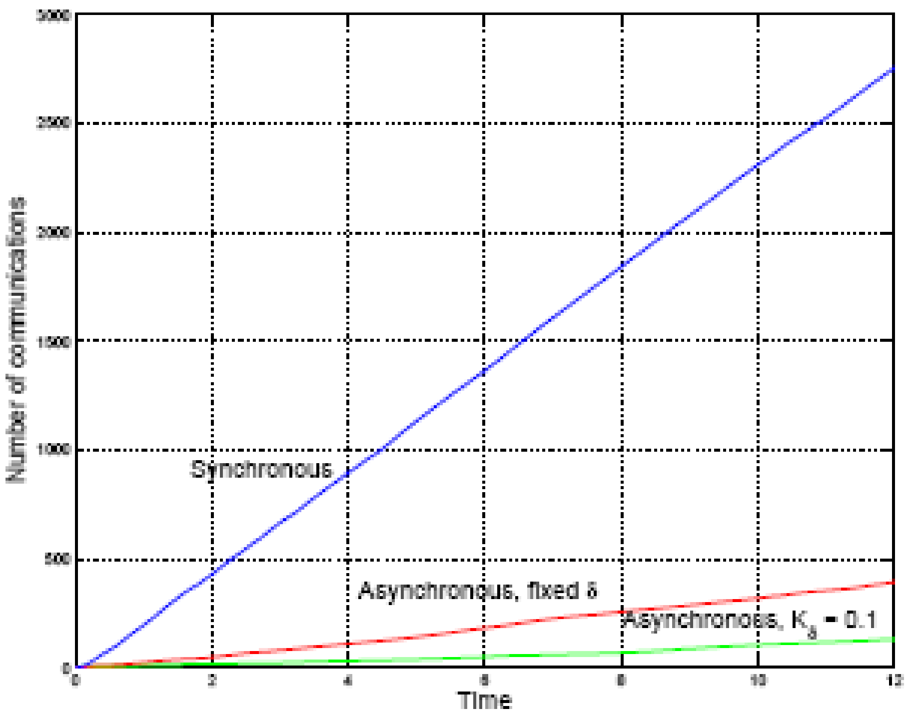
– event sources may be mobile

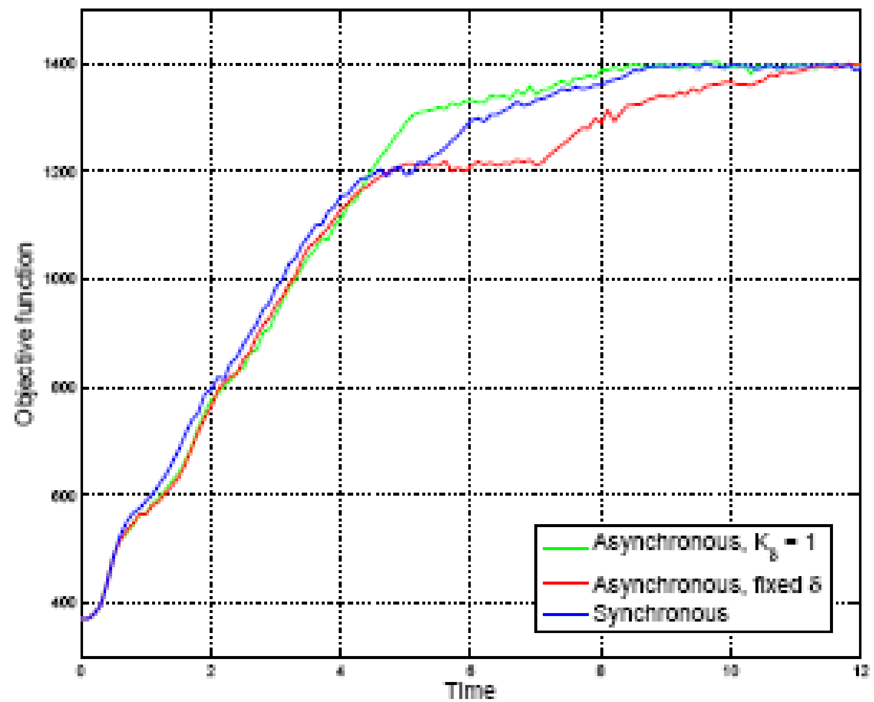
Theoretical results suggest that asynchronous communication is best.



Perceived event density over given region (mission space)

SYNCHRONOUS v ASYNCHRONOUS OPTIMIZATION PERFORMANCE





SYNCHRONOUS v ASYNCHRONOUS:

No. of communication events for a problem with *nonsmooth* gradients

SYNCHRONOUS v ASYNCHRONOUS:

Achieving optimality in a problem with *nonsmooth* gradients

Combinatorial Optimization

Butenko (Texas A&M), Vavasis (U. Waterloo), Prokopyev (U. Pittsburgh), Krokhmal (U. Iowa)

Underlying structures are often graphs; analysis is increasingly continuous non-linear optimization

Cohesive subgroups in graphs/networks

- **Data set generated by a certain complex system –**
  Represent using graphs or networks:
  Nodes = agents, Links = interactions
- **Interested in detecting cohesive (tightly knit) groups of nodes representing clusters of the system's components**
- **Earliest mathematical models of cohesive subgroups were based on the graph-theoretic concept of a clique**
- **Other subgroups include k-clubs**

Applications

- Acquaintance networks - criminal network analysis
- Wire transfer database networks - detecting money laundering
- Call networks - organized crime detection
- Protein interaction networks - predicting protein complexes
- Gene co-expression networks - detecting network motifs
- Internet graphs - information search and retrieval

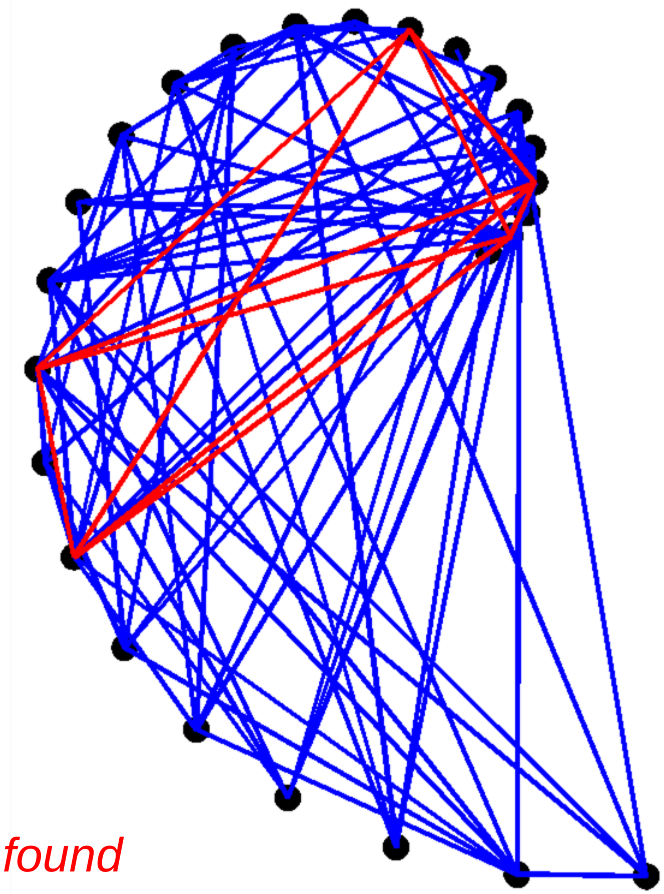
Finding hidden structures with convex optimization

U. Waterloo, S. Vavasis & H. Wolkowicz

The following random graph contains a subset of 5 nodes all mutually interconnected:

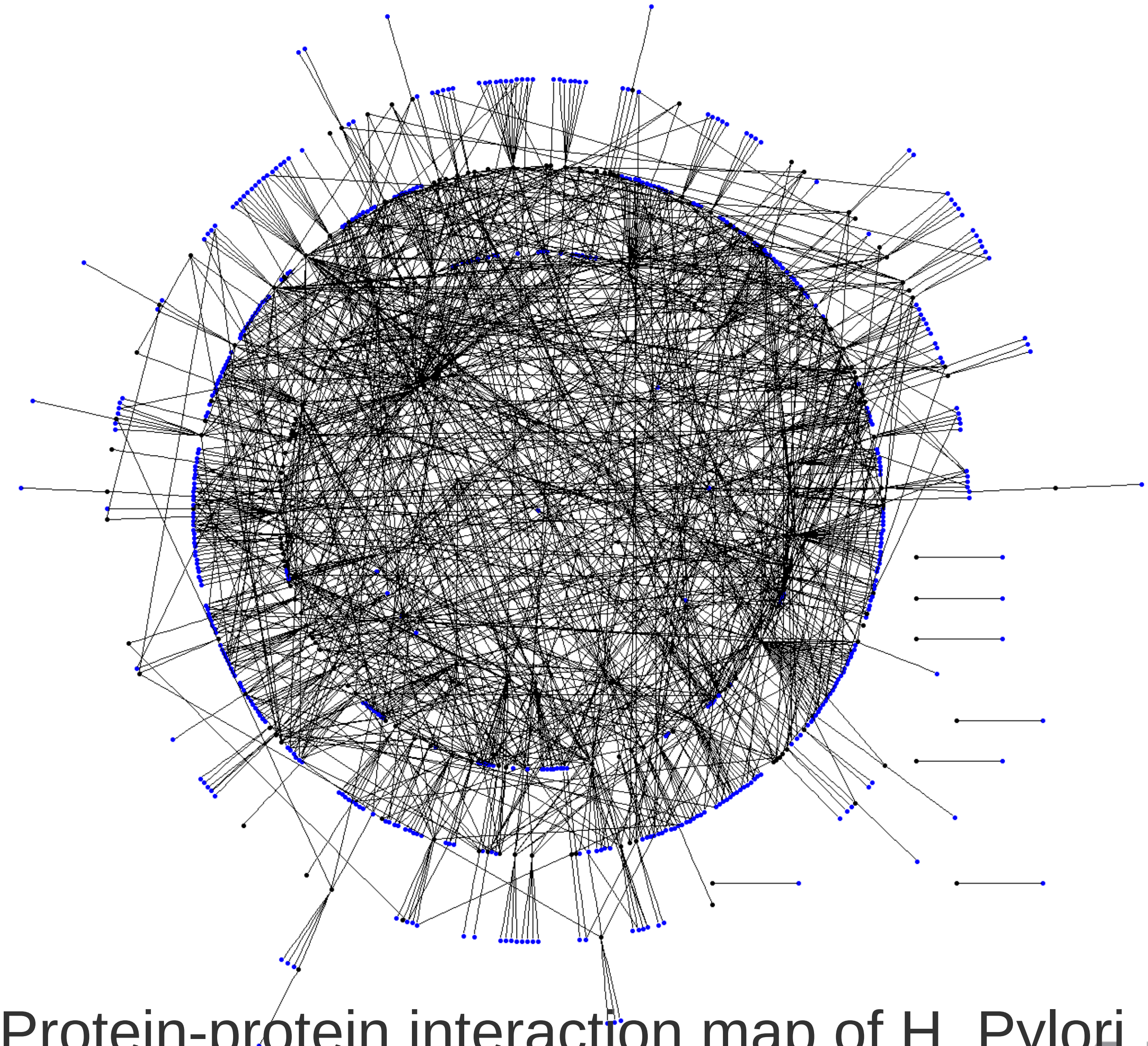
Recent data mining discoveries from Waterloo:

- Finding hidden cliques and bi-cliques in large graphs (see example)
- Finding features in images from an image database
- Clustering data in the presence of significant background noise using convex optimization



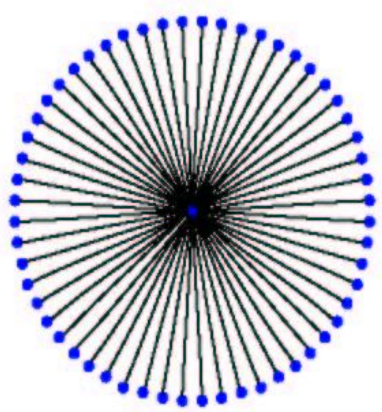
5-clique found via ***convex optimization***

Another complex network

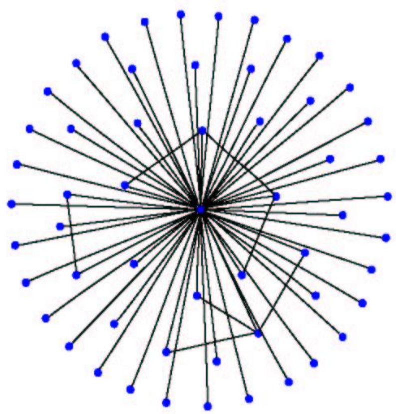


Protein-protein interaction map of H. Pylori

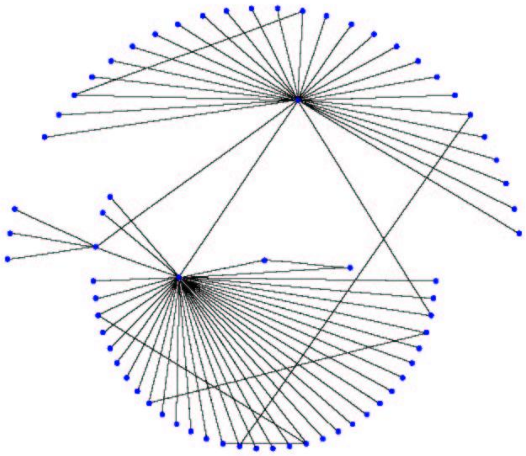
Find substructures via fractional optimization – S. Butenko, Texas A&M



Yeast – largest 2-club



H. Pylori – largest 2-club



Yeast – largest 3-club

Polyomino Tiling

U. Pittsburgh, O. Prokopyev

- **Application:**
  - **Time delay control of phased array systems**
- **Jointly supported with Dr. Nachman of AFOSR/RSE, motivated by work at the Sensors Directorate:**
  - ***Irregular Polyomino-Shaped Subarrays for Space-Based Active Arrays*** (R.J. Mailloux, S.G. Santarelli, T.M. Roberts, D. Luu)

Motivation

- **Introducing time delay into phased array systems causes significant quantization side lobes which severely degrade obtained pattern.**
- **Mailloux et al. [2006] have shown empirically that an array of `irregularly` packed polyomino-shaped subarrays has peak side lobes suppressed more than 14db when compared to an array with rectangular subarrays.**

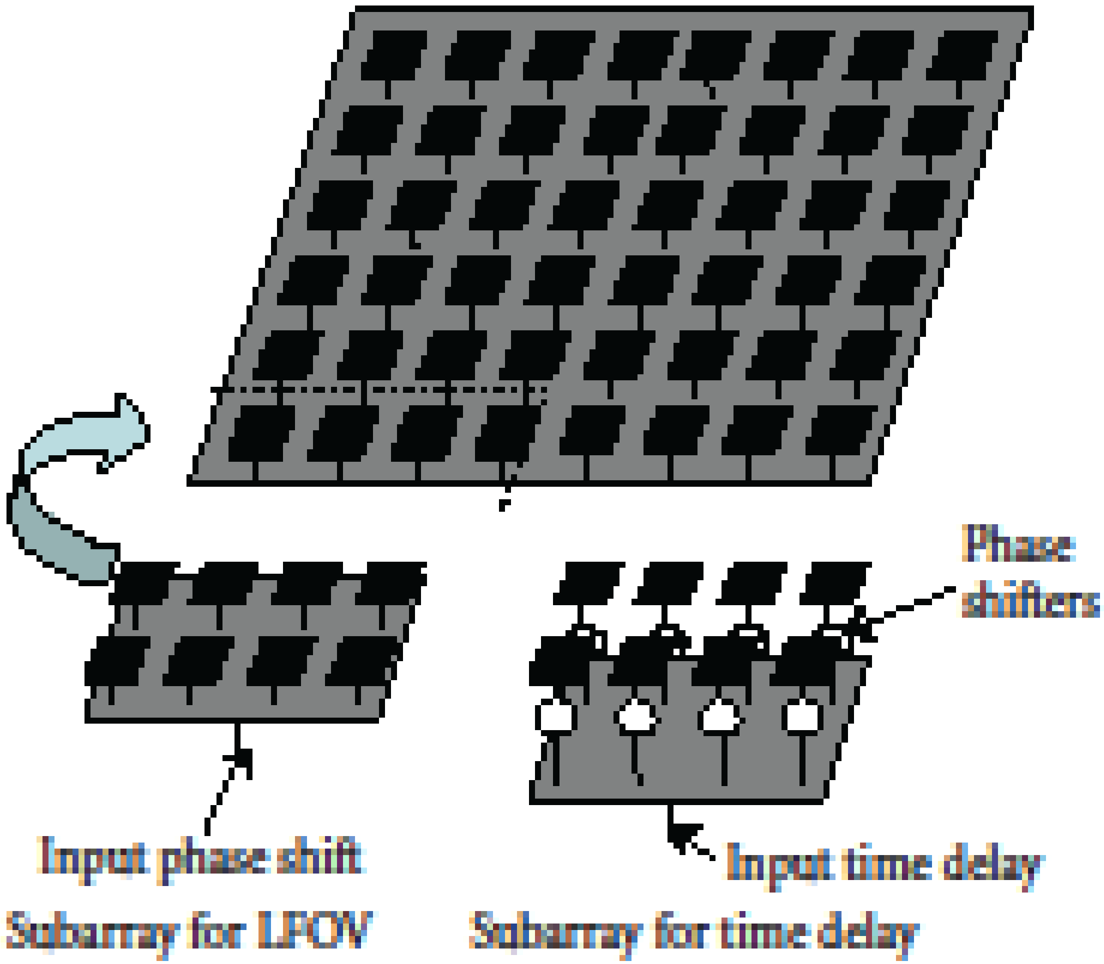


FIGURE 1: Subarray applications to LFOV and time-delayed wide-band arrays.

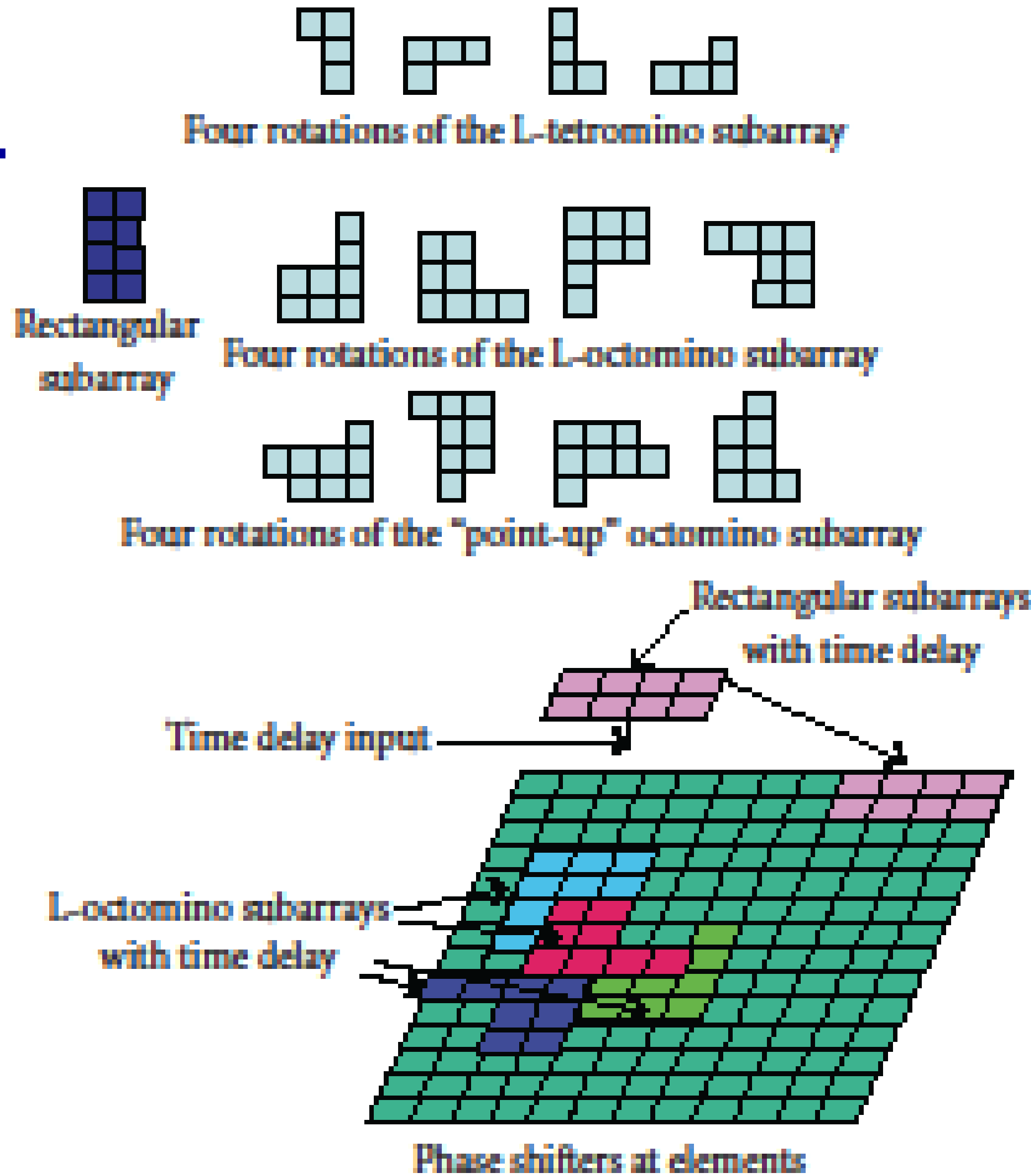
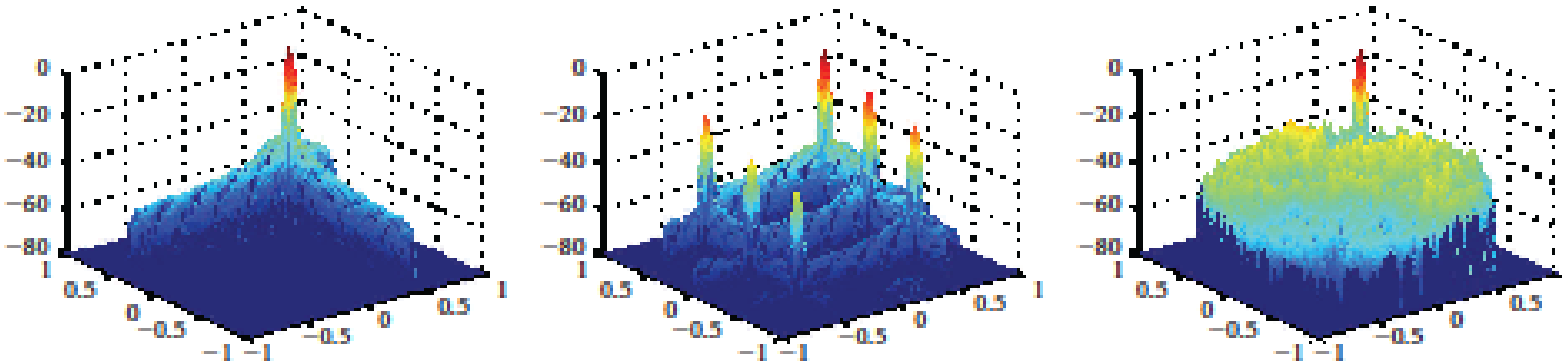


Figure 2: Irregular and rectangular subarrays.



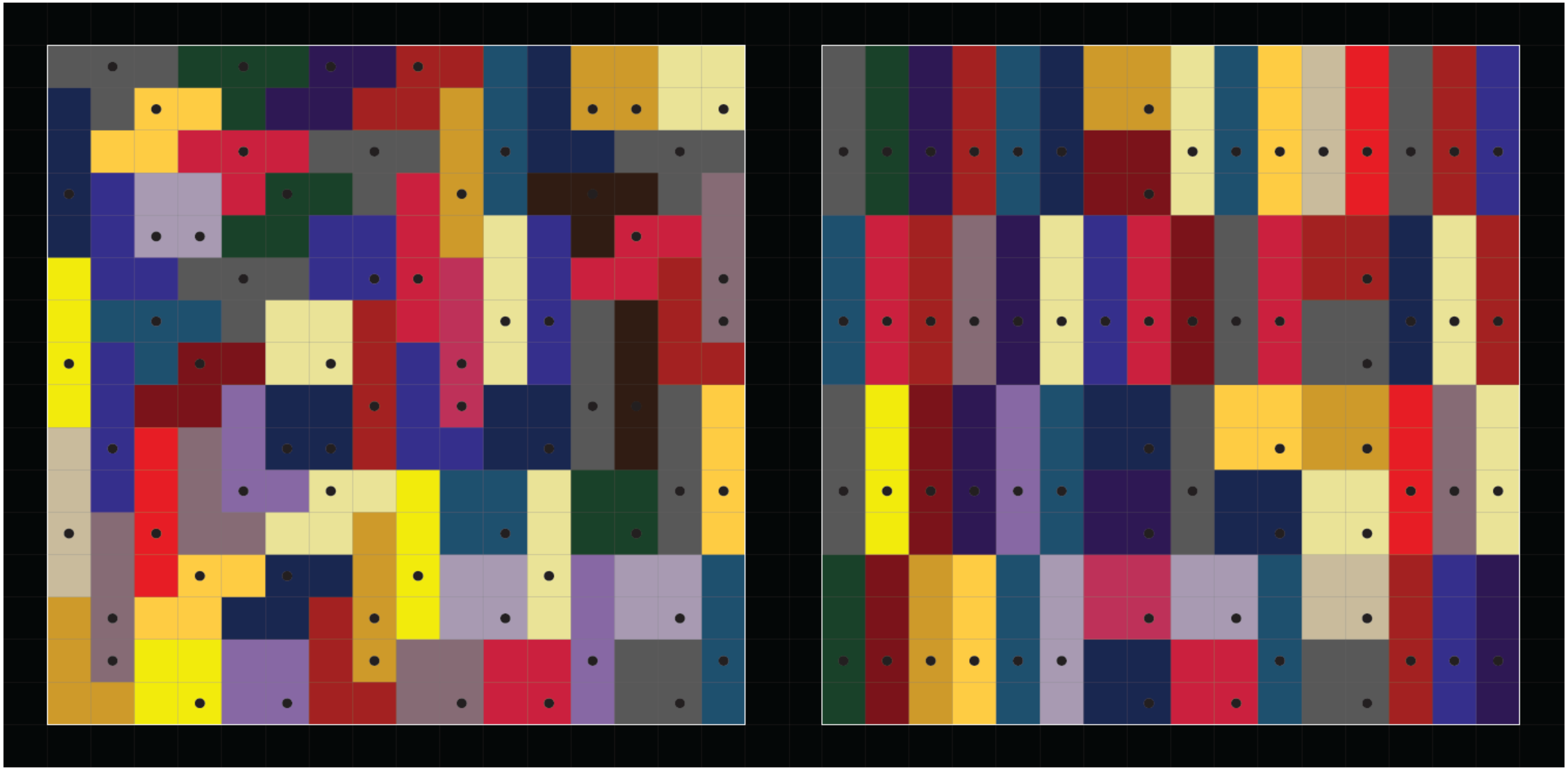
(a) (b) (c)

Figure 3: Radiation patterns at $f/f_0 = 1.3$ for an array with time delay at element level (a), at rectangular subarray inputs (b) and at L-octomino subarray inputs (c).

Initial Approach

- **The aim is to mathematically model and solve the problem of designing and arranging polyomino shaped subarrays using optimization.**
- **From information theory it is know that entropy is a measure of disorder or irregularity.**
- **How to `measure' irregularity of a given tiling of the board? Start from the concept of `center of gravity'. Every polyomino is thought as a solid and its center of gravity is found.**
- **Then, measure irregularity of the tiling by `irregularity of the centers of gravity' on the board.**
- **So the model maximizes information entropy.**

16x16 Board Tiled with Tetrominoes



Maximize entropy.

50 x 50 in 1 hr

4 Tetrominoes - 18 rotations and reflections

Minimize entropy.
(Observe how centers of gravity are aligned: order = less entropy)

Summary

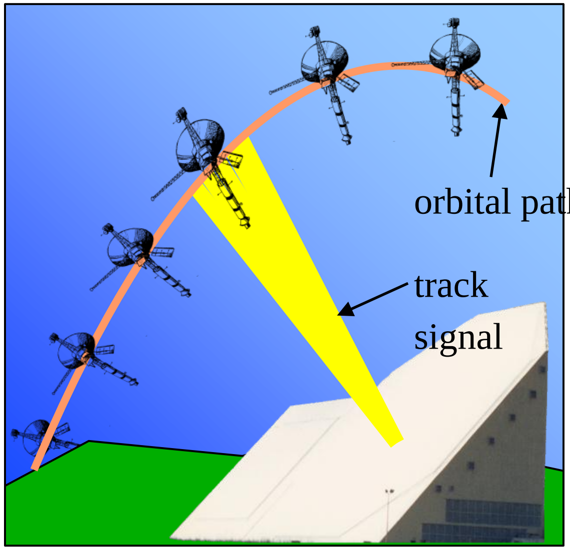
- **Goals –**
  - **Cutting edge optimization research**
  - **Of future use to the Air Force**

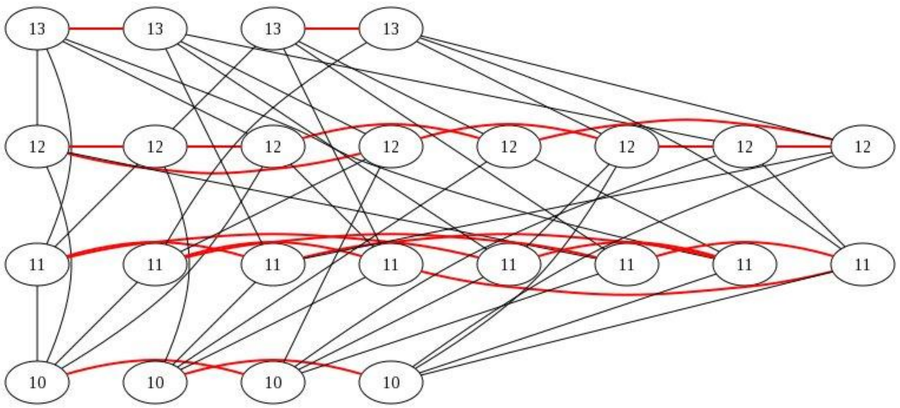
- **The primary strategy is to identify future AF applications that will require important developments in optimization theory and new algorithms.**

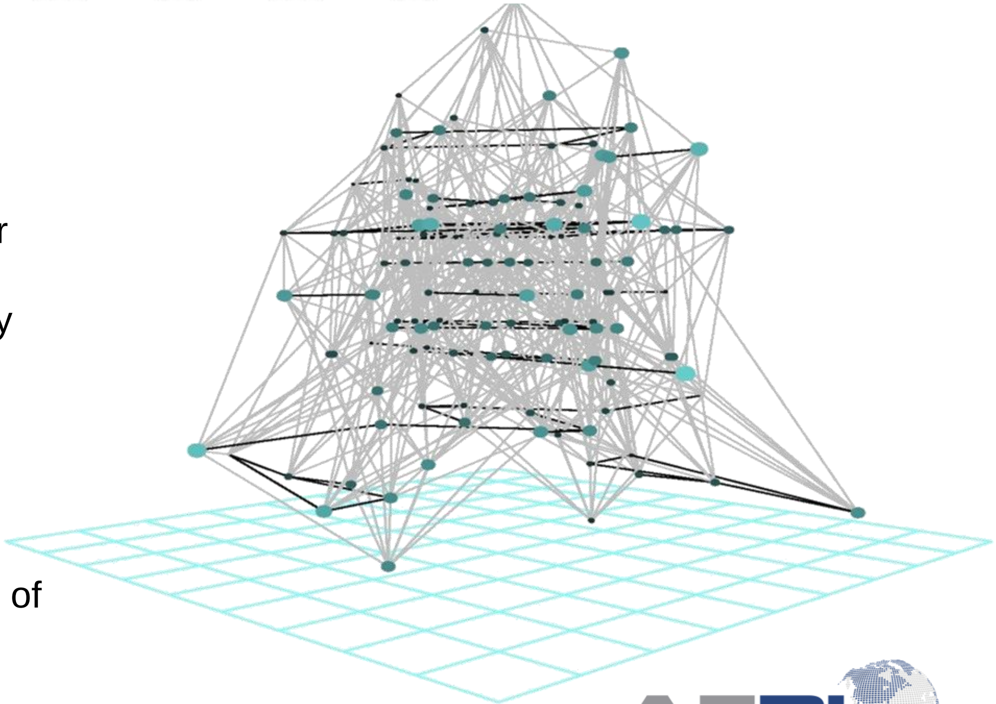
Questions?

Ongoing research: Search Algorithms for Scheduling Under Uncertainty

Colorado State University, Howe & Whitley







Approach/Technical Challenges

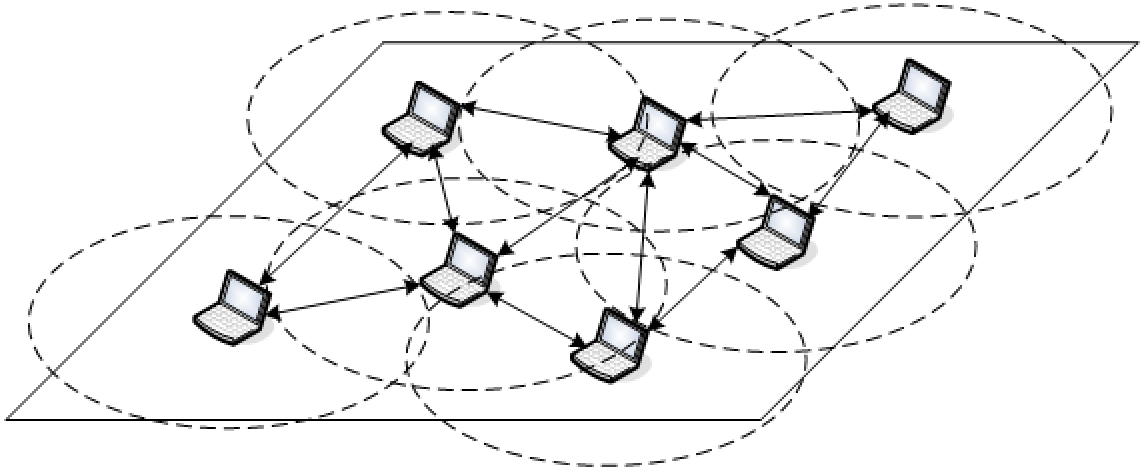
- Disconnect between theory and practice in search.
- Current theory needs to be extended to account for complex structures of real world applications.
- Uncertainty and dynamism are not well captured by current theory.

Accomplishments

- Algorithms and complexity proof for a scheduling
- Proofs about plateaus in Elementary Landscapes
- Predictive models of plateau size for some classes of landscapes based on percolation theory
- **Recent results on next slide…**

Distributed Scheduling
UIUC, R. Srikant

- **Wireless Networks:** **Links may not be able to transmit simultaneously due to interference.**
- **Collision:** **Two interfering users cannot transmit at the same time**
- **Medium Access Control (MAC) Protocol:** **Determines which links should be scheduled to transmit at each time instant.**
- ***(Relates to RSL Complex Networks portfolio)***



Main Result: The first, fully distributed algorithm which maximizes network throughput and explicitly takes interference into account.

Theoretical Contribution: An optimality proof that blends results from convex optimization, stochastic networks and mixing times of Markov chains.